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TRANSIENT COMBUSTION CALCULATIONS WITH VARIABLE THERMAL PROPERTIES

Carl W. Nelson

February 1981

US ARMY ARMAMENT RESEARCH AND DEVELOPMENT COMMAND
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The response of solid propellant combustion to steep pressurization pulses has been calculated with consideration of temperature dependent thermal properties of the solid and quasi-steady gas phase. Response has been calculated for a uniformly distributed gas phase reaction and for the Zeldovich heat feedback theory with variations in surface heat release, pressurization rate, and thermal properties of the solid.

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20. ABSTRACT (Continued)

Regression rate excursions of two to three times the quasi-steady rate ($r = aP^n$) are calculated for nominal values of propellant properties. Such excursions agree roughly with the few transient combustion measurements of Turk, et al. and Brulard, et al. Higher excursions are calculated for the distributed flame with assumed constant thermal properties. For pressurization rates approximating calculated DDT rates, the excursions survive at high pressures. Higher assumed surface heat release produces sharper response in the distributed flame models. The Zeldovich approach predicts protracted excursions from quasi-steady behavior.

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I. INTRODUCTION

Many calculations of transient solid propellant regression rates assume a quasi-steady dependence on pressure (and perhaps initial temperature). Constant volume bombs and constant pressure strand burner measurements are the usual source of the supporting data. Experiments, however, have demonstrated that in a rapidly changing pressure field, the regression rate can deviate substantially from the quasi-steady rate for increasing[1,2] or decreasing[3,4] or oscillating pressure. Because the immediate interest is in increasing pressures found in gun chambers, the body of theory and experiment for oscillating pressures will be largely ignored.

As observed in Kuo's[5] recent review, models which rely only on rate of change of pressure are valid only when the excursions are small enough for linear analysis. For larger excursions from steady state, a thermal theory model has been frequently used wherein only the gas phase is assumed quasi-steady. For extreme excursions even this approximation must be abandoned although estimates have been seriously proposed of the application limits of the quasi-steady gas.

Nelson[6] has shown that for a given gun pressurization history, calculated transient rates can vary widely with the model used. Kooker

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[1] *J. Brulard, P. Kuentzmann, R. Kling, "Réponse d'un Propergol Solide à un Echelon de Pression", La Recherche Aérospatiale, 5, 279-287 (1975).*

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[6] *C. W. Nelson, "Response of Three Types of Transient Combustion Models to Gun Pressurization", Combustion and Flame, 32, 317-319 (1978).*

and Nelson[7] showed that three thermal theory models of the KTSS[8] type give essentially the same response.

Most of these calculations assumed (1) a quasi-steady gas phase with uniform heat release and (2) constant thermal properties of both solid and gas. The uniform gas phase assumption derived from a concept of a diffusion controlled flame of composite propellants not generally held applicable to homogeneous propellants with kinetically controlled gas phase reaction. Thermal properties of the solid have been found, in the few measurements made,[9,10] to depend on temperature. The quasi-steady gas phase remains the only tractable approach for reasonable computing until methods like those of Kooker[11] can be applied to solid propellant combustion and considerably simplified. Attempts at simplified unsteady gas phase treatments tend to make critical but indefensible assumptions.[12,13]

Nelson, et al.[14] have shown that predicted pressure wave development in gun chambers is magnified by using a Zeldovich transient burning model to replace the quasi-steady regression. DDT calculations (e.g.,

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[7] *D. E. Kooker and C. W. Nelson, "Numerical Solution of Three Solid Propellant Combustion Models During a Gun Pressure Transient", USA Ballistic Research Laboratory, Report 1953 (1977). (See also ASME Journal of Heat Transfer, in press).* (AD #A035250)

[8] *H. Krier, J. S. T'ien, W. A. Sirignano and M. Summerfield, "Non-Steady Burning Phenomenon of Solid Propellants: Theory and Experiments", AIAA Journal, 6, 278-285 (1968).*

[9] *J. R. Ward, "Determination of the Heat Capacities of Gun Propellants by Differential Scanning Calorimetry", Analytical Calorimetry, 4, 143-153 (1977).*

[10] *M. L. Cohen, M. Imber "Variation of the Thermal Conductivity of Solid Propellants in an Acoustic Field", AIAA Journal 5, 1295-1299 (1967).*

[11] *D. E. Kooker, "Numerical Predictions for Laminar Flame Propagation in Confined Ozone/Oxygen Mixtures: Influence of Initial Temperature and Pressure", AIAA Paper 79-0292, New Orleans (1979).*

[12] *C. W. Nelson, "Another Comment on the Transient Burning Rate Model of Suhas and Bose", Combustion and Flame, in press.*

[13] *H. K. Suhas and T. K. Bose, "A Mathematical Model to Predict Transient Burning Rate and Pressure Decay Rates for Extinction of Composite Propellants", Combustion and Flame, 28, 145-153 (1977).*

[14] *C. W. Nelson, P. S. Gough, and F. W. Robbins, "Ignition Transients in Flamespreading Calculations", AIAA Paper 79-0166, New Orleans (1979).*

Beckstead, et al.[15]) where steep pressure fronts are well documented typically use a quasi-steady regression law.

The purpose of this short report is to examine theoretically the effect of an assumption of variable thermal properties on the transient regression rates of solid propellants.

II. THEORY

Thermal theory models solve the energy equation in the solid,

$$\rho c \frac{\partial T}{\partial t} + r\rho c \frac{\partial T}{\partial x} = \frac{\partial}{\partial x}(\lambda \frac{\partial T}{\partial x}) \quad , \tag{1}$$

which in the nondimensional variables of Kooker and Nelson[7] plus

$$L = \lambda/\lambda_o \tag{2}$$

$$C = c/c_o \tag{3}$$

becomes

$$\frac{\partial \theta}{\partial \tau} + R \frac{\partial \theta}{\partial \eta} = \frac{1}{C} \frac{\partial}{\partial \eta} (L \frac{\partial \theta}{\partial \eta}). \tag{4}$$

Boundary conditions for the solid are:

$$\theta = 0 \text{ as } \eta = -\infty \tag{5}$$

$$\frac{\partial \theta}{\partial \eta} = f[L_s, C_s, R, P(\tau)] \text{ at } \eta = 0.$$

The specific form of the surface boundary condition is set by the choice of gas phase model.

The initial condition is one of steady state burning at an initial pressure. In problems where transients seem likely to be important, the actual initial condition is a cold propellant. A complete calculation would include ignition and the transition to self-sustaining combustion.

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[15] *M. W. Beckstead, N. L. Peterson, D. T. Pilcher, and B. D. Hopkins, "Convective Combustion Modeling Applied to Deflagration to Detonation Transition of HMX", Combustion and Flame* 30, *231-241 (1977).*

Unfortunately, since there is no useful model of the transition, the problem is avoided by assuming steady state combustion has already been achieved.

At steady state, the temperature profile is given by the solution of the energy equation

$$R\frac{\partial \theta}{\partial \eta} = \frac{1}{C}\frac{\partial}{\partial \eta}\left(L\frac{\partial \theta}{\partial \eta}\right) \tag{6}$$

subject to boundary conditions

$$\theta = 0 \qquad \text{as } \eta \to -\infty$$

$$\theta = 1 \qquad \text{at } \eta = 0.$$

Note that without the temperature dependent properties, the initial condition would be the familiar

$$\theta = e^{\eta} \quad .$$

With variable properties, a numerical solution of Eq. (6) provides the initial condition.

In contrast with the constant properties case where the initial value of the surface gradient is

$$\frac{\partial \theta}{\partial \eta} = 1 \quad ,$$

the variable properties value is approximately

$$\frac{\partial \theta}{\partial \eta} = 0.65$$

for the specific values of this problem. It will in general vary from unity in the direction opposing the change in the thermal diffusivity.

One simple treatment of the gas phase is to assume a uniform reaction rate as has been done by several models (e.g., KTSS[8]). With the reaction rate so specified, the gas phase energy equation can then be integrated to find the conduction term at the solid boundary. The Kooker-Zinn[16] model here yields the boundary condition

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[16] *D. E. Kooker and B. T. Zinn, "Numerical Investigation of Nonlinear Axial Instabilities in Solid Rocket Motors", USA Ballistic Research Laboratories Contract Report 141 (1974).* (AD #776954)

$$\frac{\partial\theta}{\partial\eta} = \frac{R}{L}\left[H + (\theta_s - 1)\left(C - \frac{c_p}{c_o}\right)\right] + \frac{Zp^n}{RL} \quad .$$

The constant Z is determined from the initial condition. H is the non-dimensional surface heat release.

$$H = Q_s/c_o(T_{so} - T_o) \quad .$$

Another treatment is to ignore the gas phase details as is done in the Zeldovich approach wherein it is assumed that the functional form of the heat feedback is the same for any combination of regression rate and pressure.

For constant properties, the heat feedback term is the transformed version of the Zeldovich boundary condition,[6]

$$\frac{\partial\theta}{\partial\eta} = \frac{R}{L}\left(\theta_s - \frac{1}{\sigma_p(T_{so} - T_o)} \ln \frac{R}{R_s}\right) \quad .$$

For variable properties, the term is more complicated after considering that at steady state

$$L\frac{\partial\theta}{\partial\eta} = R\int_{\theta_o}^{\theta_s} C(\theta)d\theta \quad .$$

The essence of the Zeldovich treatment is to replace θ with an equivalent θ_{eq} to give the same regression rate-pressure relationship. For a linear heat capacity dependence ($C = C_A + C_B\theta$), the surface gradient then becomes

$$\frac{\partial\theta}{\partial\eta} = R\left[C_A(\theta_s - \theta_{eq}) + \frac{C_B}{2}(\theta_s^2 - \theta_{eq}^2)\right] \quad ,$$

where

$$\theta_{eq} = \frac{1}{\sigma_p(T_{s_o} - T_o)} \ln \frac{R}{R_s} \quad .$$

III. MEASURED THERMAL PROPERTIES

Ward[9] measured temperature dependence of heat capacity below the decomposition point for nitrocellulose and X14 propellant. For the X14 propellant the reported value was

$$C = .118 + .66\text{x}10^{-3}\ T(K)\ \text{cal/gK}$$

over the temperature range 283-343 K.

A difficulty enters here because the theory has assumed an inert solid at all temperatures. Reactions in the solid which prevent heat capacity measurement have been assumed to occur only in a collapsed zone at the surface. A simple solution is to extrapolate the measurements to the calculated temperature, however high. The alternative is a complete recasting of the model which would require knowledge of the chemical reactions in the solid.

Cohen[10] measured the thermal conductivity of two double base propellants. For DQO propellant the value is

$$\lambda = 1.90\text{x}10^{-5} + 2.46\text{x}10^{-6}\ T(K)\ \text{cal/cmsecK}$$

over the temperature range 267-317 K. Again, the simplicity of an extrapolation outweighs the more difficult alternatives.

IV. RESULTS

With the variable properties, transients are less pronounced than with constant, low temperature properties. Figure 1 shows the effect of property variation on a calculation reported by Kooker and Nelson[7] for a distributed flame. It shows that transient response is muted by the variable properties. Pressure was rising monotonically from 7 to 20 MPa during the transient as taken from the records of a 105 mm tank gun which reaches 400 MPa in about 3 ms. In Figure 1, CONCOLD means constant properties evaluated at the cold boundary; CONAVG means constant properties evaluated at an interim temperature (460 K); VAR means the variable properties.

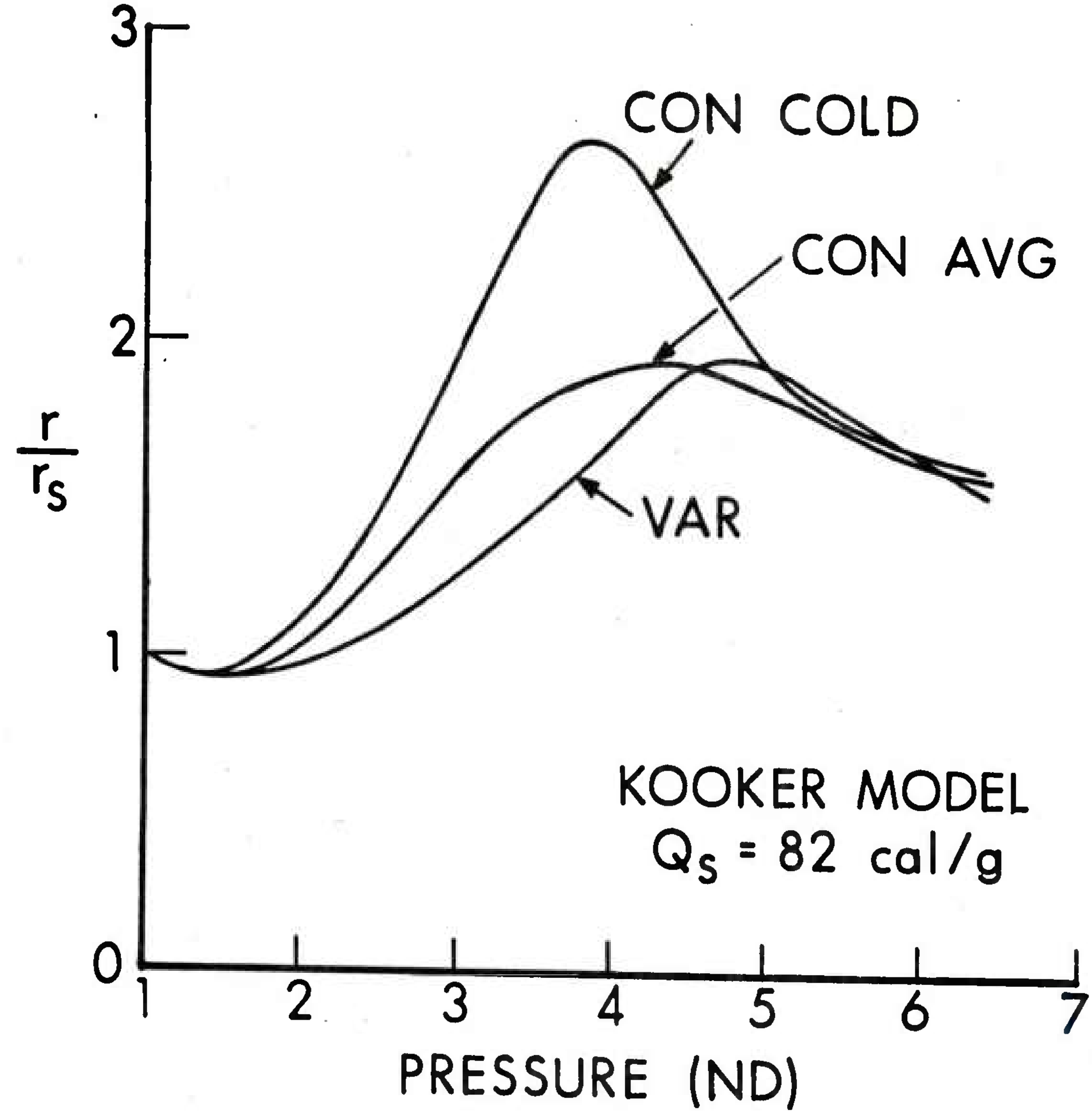

Figure 1. Effect of Variable Properties

The effect of pressurization rate on the Kooker model is shown in Figure 2. In the 105 mm tank gun, the pressurization rate at the 7-20 MPa levels is about 7000 MPa/sec. The pressurization rate of a grain during the flamespreading process in a 155 mm howitzer is calculated to be about 14,000 MPa/sec at the middle of the bed and about 40,000 MPa/sec at the stagnation of bed against the projectile base. If the Kooker flame assumptions applied, these results suggest that burning rate excursions would extend to pressures over 100 MPa. With the high pressurization rates of DDT, such an effect cannot be ignored on the assumption that the excursions apply only at low pressures.

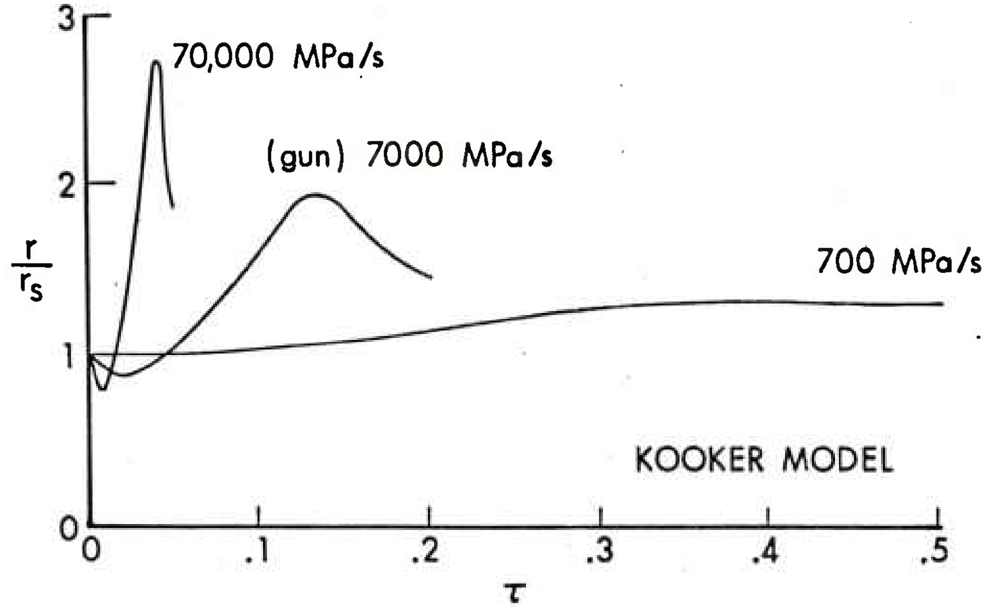

Figure 2. Effect of Pressurization Rate

Predictions of the Zeldovich model are shown in Figure 3 which shows the effect of varying temperature sensitivity and pressurization rate. Of note is the slow return of the relative rate toward unity. For the gun pressurization, an excursion of over 50% is predicted to survive for the whole ballistic cycle. With a steep pressurization rate (7×10^5 MPa/sec) the excursion is rapid on the time scale of a gun but does not peak until 50 MPa. Notable here is the transition from a lag (25% of quasi-steady rate) to an overshoot of 150% in the entire calculated cycle to a non-dimensional pressure of 173 (about 1.2 Kbars). For DDT analysis, these results say that a quasi-steady assumption ignores the predicted highly transient behavior.

Surface heat release is a critical parameter in the Kooker type model; the non-dimensional heat release is

$$H = Q_s/c_o \; (T_{s_o} - T_o) \quad .$$

The effect of varying H is shown in Figure 4. The response is similar to that of the constant properties solutions of Kooker and Nelson.[7]

Experimental values for Q_S are not well known; Kubota, et al.[17] have suggested experimental values which vary with regression rate.

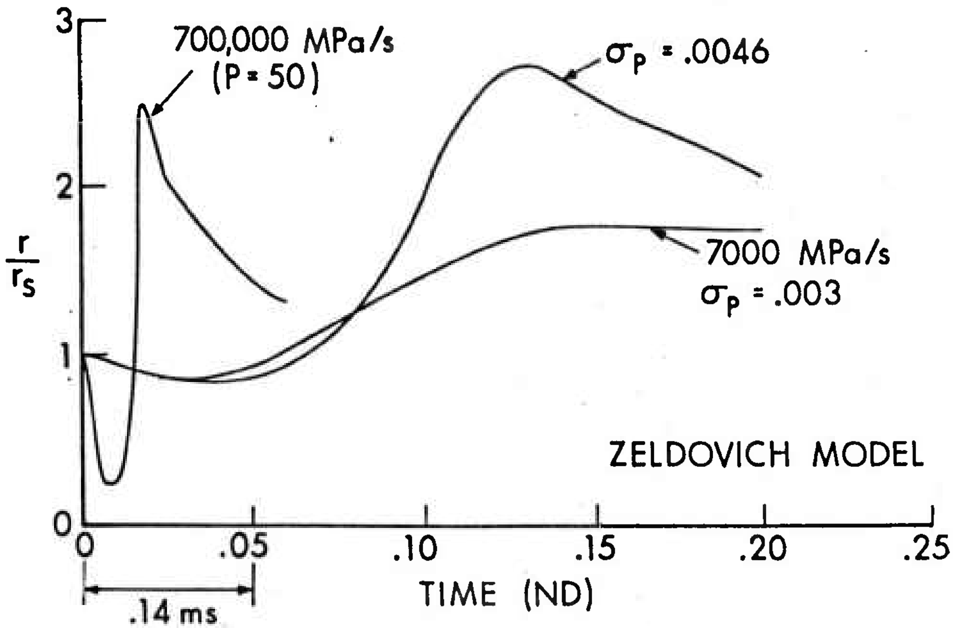

Figure 3. Zeldovich Model Results

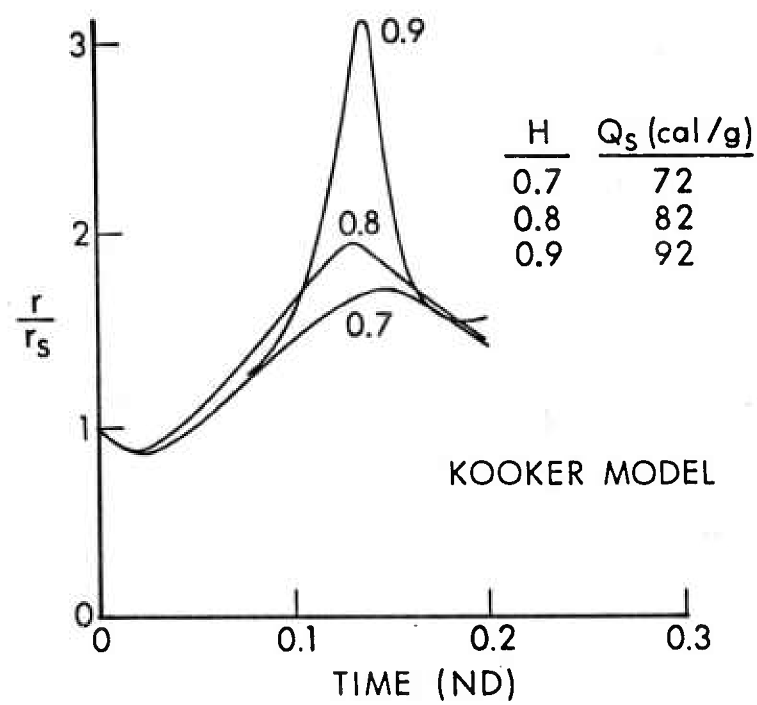

Figure 4. Effect of Surface Heat Release

The model's response to a step doubling of pressure from 1 to 2 is shown in Figure 5. Such a pressure transient represents a limit of a steep pressure wave. The step used here has no immediate practical value; it is intended only as a test of the regression rate response lag.

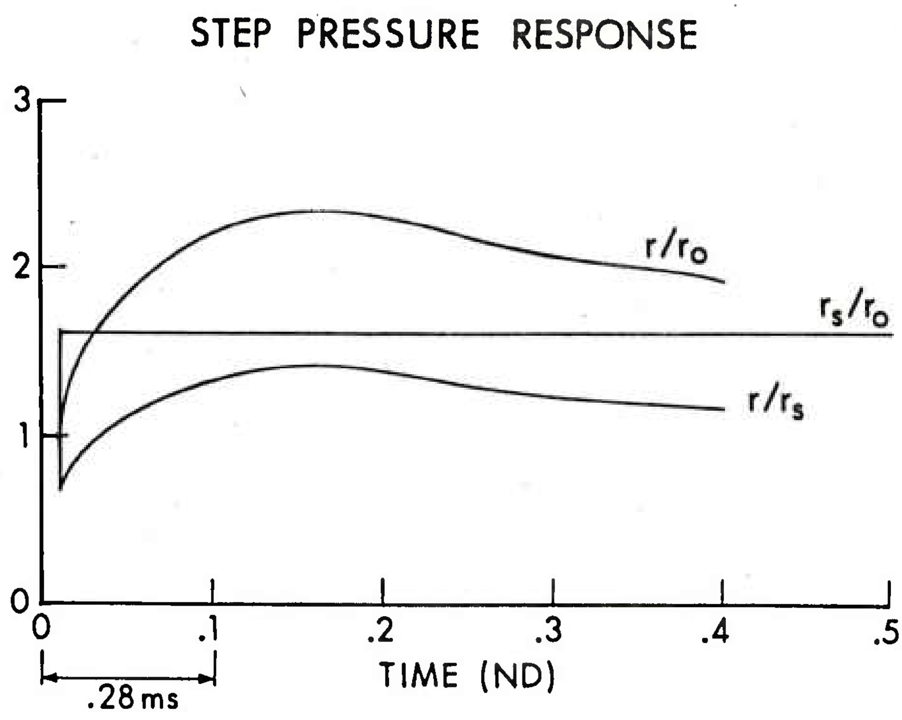

Figure 5. Effect of Pressure Step Change

CONCLUSIONS

1. The regression rate overshoots predicted with constant initial temperature thermal properties are muted by the substitution of variable thermal properties.

2. Higher pressurization rates lead to higher transients and higher pressures at the peak overshoot.

3. No simple correlation of regression rate excursion with pressurization rate.

4. Predicted excursions are dependent on assumed surface heat release.

5. Regression rate excursions of two times the quasi-steady rate are predicted.

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LIST OF SYMBOLS

C	heat capacity (nd) c/c_o
c_o	reference heat capacity
c_p	gas phase heat capacity
H	surface heat release (nd)
C_A, C_B	constants in heat capacity temperature dependence
L	conductivity (nd) λ/λ_o
P	pressure (nd) P/P_o
P_o	initial pressure
r	regression rate
R	regression rate (nd) r/r_o
r_s	steady state regression rate
r_o	initial regression rate
T	temperature
T_o	reference temperature
T_{so}	reference surface temperature
α_o	reference thermal diffusivity
η	distance (nd) xr_o/α_o
λ	thermal conductivity
λ_o	reference thermal conductivity
ρ	density
θ	temperature (nd) $(T-T_o)/T_{so}-T_o)$
σ_p	temperature sensitivity of regression rate
τ	time (nd) $t\ r_o^2/\alpha$

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